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SUBSPACE ITERATION ALGORITHMS IN FORTRAN 77 AND FORTRAN 8x

Paul J. Nikolai

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Nelson D. Wolf

FOR PAUL J. NIKOLAI
Mathematician
Design & Analysis Methods Group

Nelson D. Wolf

NELSON D. WOLF, Technical Manager
Design & Analysis Methods Group
Analysis & Optimization Branch

FOR THE COMMANDER

John T. Ach

JOHN T. ACH, Chief
Analysis & Optimization Branch
Structures Division

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This report describes a USA Fortran ANSI X3.9-1978 implementation of the Rutishauser-Reinsch subspace iteration algorithm for partial solution of the algebraic eigenvalue problem for a real matrix symmetric relative to a prescribed inner product. Also included is a corresponding description of the algorithm in the proposed Fortran 8x standard using the CFT77 compiler and the CRAY X-MP processor of Cray Research, Inc. Source code for both algorithms will be available to DOD qualified requestors in the form of a 5-1/4" diskette formatted under MS/DOS.

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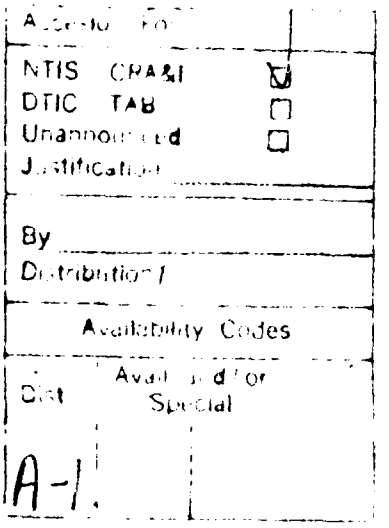
FOREWORD

This report describes work performed in the Flight Dynamics Laboratory of the U.S. Air Force Wright Aeronautical Laboratories under the Defense Research Sciences Program administered by the Air Force Office of Scientific Research under Project 2304, Mathematical and Information Sciences, and Task N1, Computational Aspects of Fluid and Structural Mechanics. It constitutes the final report for the Work Unit entitled Numerical Analysis and Machine Computations.



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I. INTRODUCTION

A previous report in this series [4] described the simultaneous or subspace iteration method for the partial solution of the generalized symmetric eigenvalue problem and provided a USA Standard Fortran X3.9 - 1966 subroutine subprogram SIMITZ implementing the algorithm. A synopsis of that report was later published in a technical journal [5] and served as a model for a Fortran X3.9 - 1978 (Fortran 77) version issued in 1983 as a component of a proprietary scientific software library distributed worldwide by Numerical Algorithms Group (NAG), Limited, of Oxford, United Kingdom. This code is referred to in the NAG Fortran Library as F02FJF [6].

The SIMITZ code as originally published proved in early experiments to be deviant in the Fortran 77 standard. Accordingly, the 1966 code has been rewritten in Fortran 77 utilizing all of the applicable features of this standard. The revised code is included with this report.

Recent experiments with the Fortran 77 version of SIMITZ have been carried out using the CFT77 compiler on a CRAY X-MP supercomputer. This compiler offers extensions to Fortran 77 some of which are part of the proposed Fortran 8x standard [3]. Accordingly, the Fortran 77 version has been rewritten to incorporate several Fortran 8x standard features, and that code is also included with this report. This new Fortran 8x version of SIMITZ exposes the algorithm for the first time to the full potential of multiple vector processors incorporating multiple functional units featured with the supercomputer offerings of Cray Research, Inc.

Section II of this report furnishes a brief mathematical description of subspace iteration. It also includes relevant implementation details and a description of test programs to enable rapid checks for correct installation. The author's recommendations comprise Section III. Finally, appendices to this report provide listings of the machine-readable documentation

furnished with each version of SIMITZ. A $5\frac{1}{4}$" diskette which includes an ASCII file of each version is provided to qualified requestors of the present report.

II. DESCRIPTION

The present programs are implementations of the subspace iteration algorithm [7] for calculating the eigenvalues largest in magnitude and corresponding eigenvectors of a real matrix symmetric relative to a prescribed inner product. Let $ip(n, w, z)$ denote an inner product in the space of real column n-tuples and let the real n-square matrix C satisfy $ip(n, Cw, z) = ip(n, w, Cz)$. Then C is *symmetric relative to ip*, and if the n-square positive definite matrix B satisfies $ip(n, w, z) = w^T Bz$ then C is *B-symmetric*. The equation $BC = C^T B$ characterizes the B-symmetry of C. Given an optional set of p initial approximate eigenvectors of a real n-square B-symmetric matrix C corresponding to p eigenvalues of C largest in magnitude, the program calculates em eigenvalues and em corresponding eigenvectors $0 \leq em < p \leq n$, to a precision dependent on the structure of C and on a prescribed tolerance eps. The matrix B is presented to the program as an independently prepared real function subprogram which calculates $ip(n, w, z) = w^T Bz$ given column n-vectors w and z. The matrix C is presented as an independently prepared subroutine subprogram $op(n, z, w)$ which when given an n-vector z computes its image $w = Cz$. The program is an outgrowth of a literal Fortran translation of the ALGOL procedure *ritzit* [8] to which it is substantially equivalent when $C = C^T$ and $ip(n, w, z) = w^T z$, the standard inner product. But depending on the choice of B and C, the present program enables the direct treatment of a wide variety of symmetric eigenproblems.

Let $A = A^T$ and $B = B^T$ denote n-square real matrices and let σ be real. If B is positive definte then the matrix $C = B^{-1}(A - \sigma B)$ is B-symmetric, and the program computes eigenvalues farthest from σ of the eigenproblem $Au = \lambda Bu$ and corresponding eigenvectors. Implementation of $op(n, z, w)$ here consists in providing for the appropriate solution for w of the linear system $Bw = (A - \sigma B)z$. Alternatively, selection of *op* to solve the system $(A - \sigma B)w = Bz$ for w enables the calculation by simultaneous inverse iteration

of the eigenvalues nearst to σ and their eigenvectors. Implications for large sparse systems for which the Cholesky factorization of B is impractical are clear.

The user may wish to supplement the following outline of the operation of the program by consulting the description of the ALGOL procedure *ritzit* in [8] as well as a review of the mathematical foundations of simultaneous iteration in [7].

Let the eigenvalues $d_1, \ldots, d_p, d_{p+1}, \ldots, d_n$ of C be arranged in order of descending absolute value and let E_p denote the direct sum of the distinct eigenspaces corresponding to $d_1, \ldots, d_p$. Let X_0 denote an n-by-p matrix having a p-dimensional column space not orthogonal relative to ip to any eigenvector in E_p. Simultaneous iteration is based on the observation that if $|d_p| > |d_{p+1}|$, the columns of the matrix $X_{k+m} = C^m X_k$ tend to a basis of E_p as $ks = k + m$ increases. But in practice all of the columns of X_k tend toward the eigenspace E_1 causing loss of information concerning the residual eigenvectors. To counter this tendency, set

$$X_{k+m} = C^m X_k R_{k+m}^{-1} \tag{1}$$

where the p-square upper triangular matrix R_{k+m} is constructed together with X_{k+m} by the Gram-Schmidt process to render the columns of X_{k+m} orthonormal relative to ip. Now the i^{th} column vector of X_k converges to the i^{th} eigenvector of C at a rate proportional to $\max_{2 \le i \le p}(|d_i/d_{i-1}|, |d_{i+1}/d_i|)$. Clearly this convergence will be delayed in the presence of eigenvalue clustering. But if $|d_p| - |d_{p+1}|$ is not too small, the column space of X_k will contain a good approximation to the i^{th} eigenvector even when k is small.

In order to recover this approximation, a modified Rayleigh-Ritz process is employed. Let Q_k denote an orthogonal matrix which diagonalizes the p-square symmetric matrix $R_k R_k^T$. Then the i^{th} column vector of

$$X_{k+1} = C X_k R_{k+1}^{-1} Q_{k+1} \tag{2}$$

coverges to the i^{th} eigenvector of C at a rate proportional to $|d_{p-1}/d_i|$ while the entries of the diagonal matrix computer with Q_k and properly ordered offer close approximations to $d_1^2, \ldots, d_p^2$. The true signed eigenvalues need only be computed at termination by diagonalizing the leading $(p-1)$-square principal submatrix of $X_k^T B C X_k$, the eigenproblem for C projected on E_{p-1} relative to ip.

The program determines a strategy for employing the devices (1) and (2) based on the distribution of the leading p eigenvalues of C upon which the convergence rate ultimately depends. The selection of values m in (1) is particularly important in this regard in that $C^m X_k$ is replaced by the m^{th} Chebychev polynomial on the interval $[-e, e]$ evaluated by a special 3-term recurrence relation and permitting accelerated convergence when values of m are continually large; e is the current value of d_p. As a result the convergence quotient lies between $|d_p/d_{em}|$ and $\exp(-\text{arccosh}\,|d_{em}/d_p|)$. It is nearer to the first value if $|d_1/d_{em}|$ is large and nearer to the second if the latter quotient is close to one.

As the iteration proceeds through a maximum of $|km|$ iteration steps -- km is a program parameter — acceptance tests for the eigenvalues and eigenvectors are conducted following each of the Rayleigh-Ritz steps (2). As soon as the relative increase of $|d_{h-1}|$ is smaller than $eps/10$, then d_{h-1} is accepted and h, the number of previously accepted eigenvalues, is increased by one. Eigenvectors are accepted in groups of one or more corresponding to clusters of accepted eigenvalues nearly equal in magnitude. If g eigenvectors have already been accepted, let $d_{g-1}, \ldots, d_\ell$ denote such a cluster. For all $j, g+1 \le j \le \ell$, denote by y_j the projection relative to ip of the image Cx_j of the j^{th} column x_j of X_k on the linear closure of $x_1, \ldots, x_\ell$. Set $f_i = \max_j ||Cx_j - y_j||/||Cx_j||$ for $i = g+1, \ldots, \ell$ where the indicated norm is the Euclidean norm or 2-norm relative to ip. If $|d_\ell| f_\ell/(|d_\ell| - e)$ is smaller than eps then all the $x_j, j = g+1, \ldots, \ell$, are accepted as eigenvectors and g is increased to ℓ. The error quantities f_i are systematically discounted in accordance with the convergence

properties of the algorithm to permit convergence in the presence of excessive round-off error or in case the parameter *eps* is prescribed unrealistically small. Having determine g eigenvectors, the iteration continues with $p - g$ remaining columns of X_k until either em eigenvectors have been calculated or kmx has been exceeded. The program may reduce em if it detects either no progress in convergence of eigenvectors corresponding to smaller eigenvalues or lack of stability in the behavior of larger eigenvalues.

The Fortran programs presented here which implement the algorithm described above differ primarily in their treatment of local storage required by SIMITZ and in the parameters associated with the procedure $op(n, z, w)$. The Fortran 77 version requires the calling program to reserve $\max(p^2, 2n) + 3p$ consecutive locations of temporary storage for use by SIMITZ. The CFT77 code tends to trade memory for speed. There temporary storage is accommodated in Fortran 8x "automatic arrays" which total $2np + p^2 + 4p$ locations and do not involve the calling program. Both versions are adapted to operate in the software environment furnished by the SLATEC Mathematical Subprogram Library [9], Version 3.1. Calling sequences are identical and agree with that of the original Fortran 66 code.

The role of the procedure $op(n, z, w)$ in the CFT77 code for the CRAY differs slightly from that in the Fortran 66 and Fortran 77 versions. In the former code z and w identify matrices of column n-vectors, and *op* must compute the image w of z under multiplication by the matrix C. Hence, *op* requires two additional parameters which identify (1) the extent of the array containing the matrix z and (2) the number of column vectors of the matrices identified by z and w. Details may be found in Appendix B. A view of what can be accomplished when *op* implements matrix multiplication by a full matrix C may be inferred from a paper of Bailey [1]. More complicated computations involving the matrices C and z require a more elaborate and careful design of the procedure *op*. A survey by Duff [2] conveys the flavor of several of these design issues when the target computer is a

multiple processor CRAY.

The Fortran 77 version of SIMITZ provided with the present report was installed and revised on a CDC CYBER 180-855 processor using the NOS 2.5 operating system and the FTN5 Fortran compiler. Subsequently, installation was carried out on a CRAY X-MP/12 processor with the COS 1.15 operating system and CFT 1.15 Fortran compiler. Revisions adhering to the Fortran 8x standard were completed with the CRAY CFT77 compiler, Version 1.3.

The revision process was accomplished in part with the aid of an executable Fortran program TESTD. Given as input the integer values n, p, and km together with a real value eps, TESTD generates a pair of random real n-square diagonal matrices A and B. It then exercises SIMITZ on the eigenvalue problem $AX - BXD = O$ where $D = diag(d_1, ..., d_p)$. For each value $em(in) = em, em = 1, ..., p - 1$, TESTD calls SIMITZ and records the number $em(r)$ of eigenpairs successfully calculated within the tolerance eps, the maximum $fmax(r)$ of the error quantities $f_i, i = 1, ..., em(r)$, and the total number $ks(r)$ of iterations expended by SIMITZ in each call. Each exercise is performed twice, once for random (r) initial eigenvectors X_0 and once when initial eigenvectors are Lanczos (ℓ) vectors [7]. TESTD finally lists the true eigenvalues, which are the diagonal entries c_i of $B^{-1}A$, and their computed counterparts d_i, the corresponding error quantities f_i and the norms e_i in the standard Euclidean metric of the residuals $(A - d_iB)X, i = 1, ..., em(\ell)$. Figure 1 shows a typical output listing from the executable program TESTD.

Fig. 1. Output List(CFT77)

N = 100 P = 10 KM = 210 EPS = 1.25E-06

EM(IN)	EM(L)	FMAX(L)	KS(L)	KS(R)	FMAX(R)	EM(R)
1	1	2.24E-08	17	30	4.13E-09	1
2	2	1.05E-07	20	30	1.87E-09	2
3	3	1.75E-07	43	50	1.55E-08	3
4	4	1.48E-07	56	56	8.45E-08	4
5	5	2.49E-07	75	75	5.36E-08	5
6	6	1.19E-07	94	75	1.14E-08	6
7	7	2.61E-07	113	138	3.51E-08	6
8	8	2.36E-07	113	138	7.71E-08	6
9	6	1.64E-07	138	138	8.10E-08	6

TOTAL KS(L) = 669 730 = TOTAL KS(R)

I	C(I)	D(I)	F(I)	E(I)
1	-1.5457629301304E+00	-1.5457629301305E+00	7.29E-08	9.84E-08
2	1.4604362516858E+00	1.4604362516858E+00	1.64E-07	2.28E-07
3	-1.1321574055138E+00	-1.1321574055138E+00	5.27E-08	5.82E-08
4	1.1042303464189E+00	1.1042303464190E+00	9.61E-10	9.55E-10
5	1.0432976702273E+00	1.0432976702274E+00	1.37E-08	1.13E-08
6	-1.0257765390463E+00	-1.0257765390463E+00	5.10E-08	3.60E-08

III. RECOMMENDATIONS

The computist having an application requiring partial solution of the large sparse symmetric eigenvalue problem now has several options. If he has access to the NAG Fortran Library, Mark 11, or to a later mark, he would do well to consider use of F02FJF from that library. The NAG version of SIMITZ has benefited by extensive independent testing by an internationally known technical staff as well as from field testing by a worldwide clientele. Moreover, a clever use of the singular value decomposition avoids the computation of the squares of the desired eigenvalues thus enhancing robustness of the code when the range of Fortran real values may be limited as on some microcomputers. This writer was unable to match the accuracy of the NAG auxiliary routines for singular value decomposition of an upper triangular matrix using the LINPACK code SSVDC found in the SLATEC collection. F02FJF may run a bit slower on some processors than its Fortran 77 SIMITZ counterpart owing to extensive subprogram calls to NAG auxiliary routines. This speed differential will decrease as the size n of the matrix increases.

If one desires to use codes which are all in the public domain, he may employ either the Fortran 77 SIMITZ or the Fortran 8x version for CRAY processors. Accuracy and robustness are almost identical owing to adherence faithfully to the ANSI standard and to the use of the SLATEC auxiliary programs.

Whichever version one uses, he should need the following advice: Gain experience with SIMITZ on problems of moderate size before investing extensive computer resources on large problems for which the codes are ultimately intended.

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APPENDIX A

Appendix A provides a listing in SLATEC format of the Fortran 77 documentation of SIMITZ.

```
C***BEGIN PROLOGUE  SIMITZ
C***DATE WRITTEN   750815   (YYMMDD)
C***REVISION DATE  881022   (YYMMDD)
C***CATAGORY NO.  F2C2, F2C9, F2D
C***KEYWORDS  EIGENVALUES,EIGENVECTORS,SUBSPACE ITERATION
C***AUTHOR  NIKOLAI, PAUL J.
C             U.S. AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
C             WRIGHT-PATTERSON AFB, OH 45433
C***PURPOSE  GIVEN AS OPTIONAL INPUT A SET OF P INITIAL APPROXIMATE
C            EIGENVECTORS OF A REAL N-SQUARE SYMMETRIC MATRIX A CORRES-
C            PONDING TO P EIGENVALUES LARGEST IN MAGNITUDE, SIMITZ COM-
C            PUTES EM EIGENVALUES LARGEST IN MAGNITUDE AND EM CORRES-
C            PONDING EIGENVECTORS TO A PRECISION DEPENDING ON THE STRUC-
C            TURE OF A AND ON A PRESCRIBED TOLERANCE EPS.  THIS VERSION
C            OF SIMITZ IS AN ANSI X3.9-1978 FORTRAN VERSION OF (1).
C***DESCRIPTION
C
C  CONTROL
C
C      DIMENSION X(LDX,P), D(P), WK(K)
C      INTEGER P, EM
C      REAL IP
C      EXTERNAL IP, INF, OP
C      .
C      .
C      .
C      CALL SIMITZ(N, P, KM, EPS, IP, OP, INF, EM, X, LDX, D, WK)
C
C  WHERE
C  N   IS AN INTEGER INPUT VARIABLE, THE ORDER OF THE MATRIX A.
C  P   IS AN INTEGER INPUT VARIABLE, THE NUMBER OF SIMULTANEOUS
C      ITERATION VECTORS.
C  KM  AS AN INTEGER INPUT VARIABLE IS IN MAGNITUDE THE MAXIMUM
C      NUMBER OF ITERATION STEPS TO BE EXECUTED.  IF KM IDENTIFIES
C      A NEGATIVE VALUE THEN P INITIAL APPROXIMATE EIGENVECTORS
C      ARE ASSUMED TO BE PRESENT IN THE ARRAY X.  OTHERWISE SIMITZ
C      SUPPLIES RANDOM INITIAL EIGENVECTORS.
C  KM  AS AN INTEGER OUTPUT VARIABLE IDENTIFIES THE NUMBER KS OF
C      ITERATION STEPS FINALLY USED IN THE CALCULATION OF EM
C      EIGENVECTORS.
C  EPS IS A REAL INPUT VARIABLE, THE TOLERANCE FOR ACCEPTING
C      EIGENVECTORS.  AS SOON AS SUCCESSIVE ITERATES OF THE RITZ
C      VALUES ABS(D(H+1)) DIFFER BY LESS THAN ABS(D(H+1))*EPS/10.0
C      THEN D(H+1) IS ACCEPTED AS AN EIGENVALUE AND H, THE NUMBER
C      OF PREVIOUSLY ACCEPTED EIGENVALUES, IS INCREASED BY 1.  AS
C      SOON AS THE ERROR QUANTITIES F(I), NORMS OF THE RESIDUALS.
C      SATISFY D(I)*F(I)/(D(I) - D(P)) .LT. EPS, THEN G, THE NUM-
C      BER OF ALREADY ACCEPTED RITZ VECTORS, IS INCREASED TO
C      G + L, I = G + 1, ..., L.  THE F(I) ARE DISCOUNTED WITH
C      SUCCESSIVE ITERATIONS TO FORCE CONVERGENCE IN CASE OF UN-
C      FORTUNATE CHOICE OF PARAMETERS.  IF M SIGNIFICANT DIGITS
C      OF ACCURACY ARE REQUIRED OF THE EIGENVALUES, THEN SET
C      EPS EQUAL TO 10.0**(-M) AS A GENERAL RULE.
C  IP  IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
```

```
C       PATIBLE REAL FUNCTION SUBPROGRAM OF THE FORM IP(N, Z, W)
C       WHICH MUST RETURN THE INNER PRODUCT OF THE VECTORS IDENTI-
C       FIED BY THE N-ARRAYS Z AND W.  WHEN A IS SYMMETRIC, IP
C       SHOULD RETURN THE STANDARD INNER PRODUCT (Z-TRANSPOSED)W.
C       WHEN A IS SYMMETRIC RELATIVE TO A GENERAL INNER PRODUCT
C       (Z-TRANSPOSED)BW, B POSITIVE DEFINITE, THEN IP MUST RETURN
C       THIS INNER PRODUCT.
C  OP   IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
C       PATIBLE SUBROUTINE SUBPROGRAM OF THE FORM OP(N, Z, W)
C       WHICH MUST CALCULATE THE IMAGE W OF THE VECTOR IDENTIFIED
C       BY THE N-ARRAY Z UNDER THE N-SQUARE MATRIX A WITHOUT OVER-
C       WRITING Z.
C  INF  IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
C       PATIBLE SUBROUTINE SUBPROGRAM WHICH MAY BE USED FOR
C       OBTAINING INFORMATION OR TO EXERT CONTROL DURING EXECUTION
C       OF SIMITZ.  INF HAS THE FORM INF(KS, G, H, F) WHERE
C         KS IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF THE NEXT
C            ITERATION STEP.
C         G  IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF ALREADY
C            ACCEPTED EIGENVECTORS.
C         H  IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF ALREADY
C            ACCEPTED EIGENVALUES.
C         F  IS A REAL OUTPUT VARIABLE P-ARRAY, ERROR QUANTITIES
C            MEASURING RESPECTIVELY THE STATE OF CONVERGENCE OF
C            THE P SIMULTANEOUS ITERATION VECTORS.  EACH ELEMENT OF
C            THE ARRAY F IS INITIALLY SET BY SIMITZ TO THE VALUE 4.0.
C  EM   AS AN INTEGER INPUT VARIABLE IS THE NUMBER OF EIGENVALUES
C       TO BE COMPUTED, 0 .LT. EM .LT. P .LE. N .LE. LDX.
C  EM   AS AN INTEGER OUTPUT VARIABLE IS THE NUMBER OF EIGENVECTORS
C       COMPUTED THROUGH KM ITERATION STEPS.
C  X    AS A REAL N-BY-P INPUT ARRAY IS A SET OF P OPTIONAL INITIAL
C       APPROXIMATE EIGENVECTORS X(I,1), ..., X(I,P), I = 1, ...,
C       N, INTERPRETED BY SIMITZ IF KM IS NEGATIVE.
C  X    AS A REAL N-BY-P OUTPUT ARRAY IS A SET OF EM EIGENVECTORS
C       X(I,1), ..., X(I,EM), I = 1, ..., N, COMPUTED THROUGH
C       ABS(KM) ITERATION STEPS WITH THE REMAINDER OF X CONSISTING
C       OF P - EM APPROXIMATE EIGENVECTORS.  THE P-SQUARE MATRIX
C       WHOSE (J, L) ENTRY IS IP(N, X(1,J), X(1,L)) IS THE IDEN-
C       TITY MATRIX; THAT IS, THE EIGENVECTORS OF A ARE ORTHO-
C       NORMAL RELATIVE TO THE INNER PRODUCT IP.
C  LDX  IS AN INTEGER INPUT VARIABLE WHICH IDENTIFIES THE LEADING
C       DIMENSION IN THE CALLING PROGRAM OF THE ARRAY X.
C  D    IS A REAL OUTPUT P-ARRAY OF WHICH D(1), ..., D(EM) ARE THE
C       EIGENVALUES OF A LARGEST IN MAGNITUDE IN DECREASING ORDER
C       CORRESPONDING TO THE COMPUTED EIGENVECTORS X(I,1), ...,
C       X(I,EM), I = 1, ..., N.  D(EM+1), ..., D(P-1) CONTAIN
C       APPROXIMATIONS TO PROGRESSIVELY SMALLER SUCH EIGENVALUES.
C       D(P) CONTAINS THE MOST RECENTLY COMPUTED VALUE OF E, WHERE
C       THE INTERVAL (-E, E) IS THE INTERVAL OVER WHICH THE
C       CHEBYSHEV ACCELERATION WAS PERFORMED.
C  WK   THE INITIAL LOCATION OF AT LEAST MAX(P**2, 2*N) + 3*P = K
C       CONSECUTIVE STORAGE LOCATIONS WHICH MAY NOT BE OVER-
C       WRITTEN WHILE SIMITZ IS IN EXECUTION.
C
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C  OTHER PROGRAMMING INFORMATION
C
C  THIS VERSION OF SIMITZ IS DESIGNED TO OPERATE IN THE SOFTWARE
C  ENVIRONMENT FURNISHED BY THE SLATEC COLLECTION, VERSION 3.1.
C
C  THE PERFORMANCE OF SIMITZ IS STRONGLY DEPENDENT UPON THE CHOICE
C  OF INPUT PARAMETERS AND UPON THE CAREFUL PREPARATION OF THE
C  SUBPROGRAMS IP AND OP.  THE USER SHOULD CONSIDER USING HIS OWN
C  ACTIVE SUBROUTINE INF TO MONITOR PROGRESS OF SIMITZ RELATIVE TO
C  HIS CHOICE OF INPUT PARAMETERS IF NO INFORMATION IS OTHERWISE
C  AVAILABLE CONCERNING THE LOCATIONS OF THE RELEVANT EIGENVALUES.
C  RECALL THAT SIMITZ MAY BE REENTERED WITH KM .LT. 0 WITHOUT LOSS
C  OF INFORMATION TO PERMIT CONSERVATIVE INITIAL CHOICES OF
C  ABS(KM), EPS AND P.
C
C  OTHER PROGRAMS REQUIRED
C
C     FUNCTION RAND
C         RETURNS UNIFORMLY DISTRIBUTED RANDOM NUMBERS ON THE OPEN
C         INTERVAL (0, 1).
C     SUBROUTINE TRED2
C         IS THE EISPACK (4) PROGRAM WHICH COMPUTES A HOUSEHOLDER
C         TRIDIAGONAL FORM OF A REAL SYMMETRIC MATRIX.
C     SUBROUTINE IMTQL2
C         IS THE EISPACK PROGRAM WHICH COMPUTES THE EIGENVALUES AND
C         ORTHONORMAL EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX.
C     SUBROUTINE XERRWV
C         PROCESSES AN ERROR (DIAGNOSTIC) MESSAGE.
C     FUNCTION R1MACH
C         RETURNS SINGLE PRECISION MACHINE DEPENDENT CONSTANTS.
C     FUNCTION IP
C         IS DESCRIBED ABOVE.
C     SUBROUTINE OP
C         IS DESCRIBED ABOVE.
C     SUBROUTINE INF
C         IS DESCRIBED ABOVE.
C
C  METHOD
C
C     SIMITZ REPRESENTS RESULTS OF EXTENSIVE MODIFICATIONS AND TESTS
C     OF SUBROUTINE SIMITZ (1), A FORTRAN 66 TRANSLATION OF THE
C     ALGOL 60 PROCEDURE RITZIT (3).  THE BASIC RUTISHAUSER-REINSCH
C     ALGORITHM IS PRESERVED.
C***REFERENCES  (1) PAUL J. NIKOLAI, ALGORITHM 538 - EIGENVECTORS AND
C                   EIGENVALUES OF REAL GENERALIZED SYMMETRIC MATRICES BY
C                   SIMULTANEOUS ITERATION, ACM TRANS. MATH. SOFTWARE 5
C                   (1979), 118-125.
C                 (2) BERESFORD N. PARLETT, THE SYMMETRIC EIGENVALUE
C                   PROBLEM, PRENTICE-HALL, ENGLEWOOD CLIFFS, 1930.
C                 (3) HEINZ RUTISHAUSER, SIMULTANEOUS ITERATION METHOD FOR
C                   SYMMETRIC MATRICES, NUMER. MATH. 16(1970), 205-223.
C                 (4) B.T. SMITH ET AL, MATRIX EIGENSYSTEM ROUTINES -
C                   EISPACK GUIDE, 2-ND ED.,LECTURE NOTES IN COMPUTER
C                   SCIENCE 6, SPRINGER-VERLAG, NEW YORK, 1976.
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C***ROUTINES CALLED  IMTQL2,R1MACH,RAND,TRED2,XERRWV
C***END PROLOGUE
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APPENDIX B

Appendix B provides a listing in SLATEC format of the Fortran 8x documentation of SIMITZ.

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C***BEGIN PROLOGUE  SIMITZ
C***DATE WRITTEN   750815   (YYMMDD)
C***REVISION DATE  881115   (YYMMDD)
C***CATAGORY NO.  F2C2, F2C9, F2D
C***KEYWORDS  EIGENVALUES,EIGENVECTORS,SUBSPACE ITERATION
C***AUTHOR  NIKOLAI, PAUL J.
C             U.S. AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
C             WRIGHT-PATTERSON AFB, OH 45433
C***PURPOSE  GIVEN AS OPTIONAL INPUT A SET OF P INITIAL APPROXIMATE
C            EIGENVECTORS OF A REAL N-SQUARE SYMMETRIC MATRIX A CORRES-
C            PONDING TO P EIGENVALUES LARGEST IN MAGNITUDE, SIMITZ COM-
C            PUTES EM EIGENVALUES LARGEST IN MAGNITUDE AND EM CORRES-
C            PONDING EIGENVECTORS TO A PRECISION DEPENDING ON THE STRUC-
C            TURE OF A AND ON A PRESCRIBED TOLERANCE EPS.  THIS VERSION
C            OF SIMITZ IS A CRAY CFT77 FORTRAN VERSION OF (1).
C***DESCRIPTION
C
C  CONTROL
C
C       REAL X(LDX,P), D(P)
C       INTEGER P, EM
C       REAL IP
C       EXTERNAL IP, INF, OP
C       .
C       .
C       .
C       CALL SIMITZ(N, P, KM, EPS, IP, OP, INF, EM, X, LDX, D, WK)
C
C  WHERE
C  N    IS AN INTEGER INPUT VARIABLE, THE ORDER OF THE MATRIX A.
C  P    IS AN INTEGER INPUT VARIABLE, THE NUMBER OF SIMULTANEOUS
C       ITERATION VECTORS.
C  KM   AS AN INTEGER INPUT VARIABLE IS IN MAGNITUDE THE MAXIMUM
C       NUMBER OF ITERATION STEPS TO BE EXECUTED.  IF KM IDENTIFIES
C       A NEGATIVE VALUE THEN P INITIAL APPROXIMATE EIGENVECTORS
C       ARE ASSUMED TO BE PRESENT IN THE ARRAY X.  OTHERWISE SIMITZ
C       SUPPLIES RANDOM INITIAL EIGENVECTORS.
C  KM   AS AN INTEGER OUTPUT VARIABLE IDENTIFIES THE NUMBER KS OF
C       ITERATION STEPS FINALLY USED IN THE CALCULATION OF EM
C       EIGENVECTORS.
C  EPS  IS A REAL INPUT VARIABLE, THE TOLERANCE FOR ACCEPTING
C       EIGENVECTORS.  AS SOON AS SUCCESSIVE ITERATES OF THE RITZ
C       VALUES ABS(D(H+1)) DIFFER BY LESS THAN ABS(D(H+1))*EPS/10.0
C       THEN D(H+1) IS ACCEPTED AS AN EIGENVALUE AND H, THE NUMBER
C       OF PREVIOUSLY ACCEPTED EIGENVALUES, IS INCREASED BY 1.  AS
C       SOON AS THE ERROR QUANTITIES F(I), NORMS OF THE RESIDUALS,
C       SATISFY D(I)*F(I)/(D(I) - D(P)) .LT. EPS, THEN G, THE NUM-
C       BER OF ALREADY ACCEPTED RITZ VECTORS, IS INCREASED TO
C       G + L, I = G + 1, ..., L.  THE F(I) ARE DISCOUNTED WITH
C       SUCCESSIVE ITERATIONS TO FORCE CONVERGENCE IN CASE OF UN-
C       FORTUNATE CHOICE OF PARAMETERS.  IF M SIGNIFICANT DIGITS
C       OF ACCURACY ARE REQUIRED OF THE EIGENVALUES, THEN SET
C       EPS EQUAL TO 10.0**(-M) AS A GENERAL RULE.
C  IP   IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
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C       PATIBLE REAL FUNCTION SUBPROGRAM OF THE FORM IP(N, Z, W)
C       WHICH MUST RETURN THE INNER PRODUCT OF THE VECTORS IDENTI-
C       FIED BY THE N ARRAYS Z AND W.  WHEN A IS SYMMETRIC, IP
C       SHOULD RETURN THE STANDARD INNER PRODUCT (Z-TRANSPOSED)W.
C       WHEN A IS SYMMETRIC RELATIVE TO A GENERAL INNER PRODUCT
C       (Z-TRANSPOSED)BW, B POSITIVE DEFINITE, THEN IP MUST RETURN
C       THIS INNER PRODUCT.
C  OP   IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
C       PATIBLE SUBROUTINE SUBPROGRAM OF THE FORM OP(N, Z, LDZ, W, M)
C       WHICH MUST CALCULATE THE IMAGE W OF THE N-BY-M MATRIX IDENTI-
C       FIED BY THE LDZ-BY-M ARRAY Z UNDER THE N-SQUARE MATRIX A WITH-
C       OUT OVERWRITING Z.  SUBROUTINE OP(N, Z, LDZ, W, M) MUST INCLUDE
C       SPECIFICATION STATEMENTS EQUIVALENT TO: REAL Z(LDZ, M) , W(N, M)
C  INF  IS AN EXTERNAL INPUT VARIABLE, THE NAME OF A FORTRAN COM-
C       PATIBLE SUBROUTINE SUBPROGRAM WHICH MAY BE USED FOR
C       OBTAINING INFORMATION OR TO EXERT CONTROL DURING EXECUTION
C       OF SIMITZ.  INF HAS THE FORM INF(KS, G, H, F) WHERE
C         KS IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF THE NEXT
C            ITERATION STEP.
C         G  IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF ALREADY
C            ACCEPTED EIGENVECTORS.
C         H  IS AN INTEGER OUTPUT VARIABLE, THE NUMBER OF ALREADY
C            ACCEPTED EIGENVALUES.
C         F  IS A REAL OUTPUT VARIABLE P-ARRAY, ERROR QUANTITIES
C            MEASURING RESPECTIVELY THE STATE OF CONVERGENCE OF
C            THE P SIMULTANEOUS ITERATION VECTORS.  EACH ELEMENT OF
C            THE ARRAY F IS INITIALLY SET BY SIMITZ TO THE VALUE 4.0.
C  EM   AS AN INTEGER INPUT VARIABLE IS THE NUMBER OF EIGENVALUES
C       TO BE COMPUTED, 0 .LT. EM .LT. P .LE. N .LE. LDX.
C  EM   AS AN INTEGER OUTPUT VARIABLE IS THE NUMBER OF EIGENVECTORS
C       COMPUTED THROUGH KM ITERATION STEPS.
C  X    AS A REAL N-BY-P INPUT ARRAY IS A SET OF P OPTIONAL INITIAL
C       APPROXIMATE EIGENVECTORS X(I,1), ..., X(I,P), I = 1, ...,
C       N, INTERPRETED BY SIMITZ IF KM IS NEGATIVE.
C  X    AS A REAL N-BY-P OUTPUT ARRAY IS A SET OF EM EIGENVECTORS
C       X(I,1), ..., X(I,EM), I = 1, ..., N, COMPUTED THROUGH
C       ABS(KM) ITERATION STEPS WITH THE REMAINDER OF X CONSISTING
C       OF P - EM APPROXIMATE EIGENVECTORS.  THE P-SQUARE MATRIX
C       WHOSE (J, L) ENTRY IS IP(N, X(1,J), X(1,L)) IS THE IDEN-
C       TITY MATRIX; THAT IS, THE EIGENVECTORS OF A ARE ORTHO-
C       NORMAL RELATIVE TO THE INNER PRODUCT IP.
C  LDX  IS AN INTEGER INPUT VARIABLE, THE EXTENT IN THE LEADING
C       DIMENSION OF THE ARRAY X IN THE CALLING PROGRAM.
C  D    IS A REAL OUTPUT P-ARRAY OF WHICH D(1), ..., D(EM) ARE THE
C       EIGENVALUES OF A LARGEST IN MAGNITUDE IN DECREASING ORDER
C       CORRESPONDING TO THE COMPUTED EIGENVECTORS X(I,1), ...,
C       X(I,EM), I = 1, ..., N.  D(EM+1), ..., D(P-1) CONTAIN
C       APPROXIMATIONS TO PROGRESSIVELY SMALLER SUCH EIGENVALUES.
C       D(P) CONTAINS THE MOST RECENTLY COMPUTED VALUE OF E, WHERE
C       THE INTERVAL (-E, E) IS THE INTERVAL OVER WHICH THE
C       CHEBYSHEV ACCELERATION WAS PERFORMED.
C  WK   IS A REAL INPUT VARIABLE UNUSED BY SUBROUTINE SIMITZ.  WK IS
C       INCLUDED ONLY FOR COMPATIBILITY WITH PREVIOUS VERSIONS.
C       WORKING STORAGE IS ACCOMMODATED BY AUTOMATIC ARRAYS WITHIN
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C      SIMITZ.
C
C  OTHER PROGRAMMING INFORMATION
C
C  THIS VERSION OF SIMITZ IS DESIGNED TO OPERATE IN THE SOFTWARE
C  ENVIRONMENT FURNISHED BY THE SLATEC MATHEMATICAL SUBPROGRAM LIBRARY,
C  VERSION 3.1.
C
C  THE PERFORMANCE OF SIMITZ IS STRONGLY DEPENDENT UPON THE CHOICE
C  OF INPUT PARAMETERS AND UPON THE CAREFUL PREPARATION OF THE
C  SUBPROGRAMS IP AND OP.  THE USER SHOULD CONSIDER USING HIS OWN
C  ACTIVE SUBROUTINE INF TO MONITOR PROGRESS OF SIMITZ RELATIVE TO
C  HIS CHOICE OF INPUT PARAMETERS IF NO INFORMATION IS OTHERWISE
C  AVAILABLE CONCERNING THE LOCATIONS OF THE RELEVANT EIGENVALUES.
C  RECALL THAT SIMITZ MAY BE REENTERED WITH KM .LT. 0 WITHOUT LOSS
C  OF INFORMATION TO PERMIT CONSERVATIVE INITIAL CHOICES OF
C  ABS(KM), EPS AND P.
C
C  OTHER PROGRAMS REQUIRED
C
C     SUBROUTINE ORTHOG - SUBSIDIARY SUBPROGRAM
C         PERFORMS ORTHONORMALIZATION RELATIVE TO THE REAL INNER
C         PRODUCT IP BY THE GRAM-SCHMIDT PROCESS OF THE TERMINAL
C         COLUMN VECTORS OF THE MATRIX X GIVEN THAT THE INITIAL
C         COLUMNS ARE IP ORTHONORMAL.
C     SUBROUTINE RANDOM - SUBSIDIARY SUBPROGRAM
C         INSERTS UNIFORMLY DISTRIBUTED RANDOM REAL VALUES FROM THE
C         INTERVAL (-1, 1) INTO COLUMN VECTORS OF THE MATRIX X.
C     SUBROUTINE TRED2
C         IS THE EISPACK (4) PROGRAM WHICH COMPUTES A HOUSEHOLDER
C         TRIDIAGONAL FORM OF A REAL SYMMETRIC MATRIX.
C     SUBROUTINE IMTQL2
C         IS THE EISPACK PROGRAM WHICH COMPUTES THE EIGENVALUES AND
C         ORTHONORMAL EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX.
C     SUBROUTINE XERRWV
C         PROCESSES AN ERROR (DIAGNOSTIC) MESSAGE.
C     FUNCTION R1MACH
C         RETURNS SINGLE PRECISION MACHINE DEPENDENT CONSTANTS.
C     FUNCTION IP
C         IS DESCRIBED ABOVE.
C     SUBROUTINE OP
C         IS DESCRIBED ABOVE.
C     SUBROUTINE INF
C         IS DESCRIBED ABOVE.
C
C  METHOD
C
C     SIMITZ REPRESENTS RESULTS OF EXTENSIVE MODIFICATIONS AND TESTS
C     OF SUBROUTINE SIMITZ (1), A FORTRAN 66 TRANSLATION OF THE
C     ALGOL 60 PROCEDURE RITZIT (3).  THE BASIC RUTISHAUSER-REINSCH
C     ALGORITHM IS PRESERVED.
C***REFERENCES  (1) PAUL J. NIKOLAI, ALGORITHM 538 - EIGENVECTORS AND
C                   EIGENVALUES OF REAL GENERALIZED SYMMETRIC MATRICES BY
C                   SIMULTANEOUS ITERATION, ACM TRANS. MATH. SOFTWARE 5
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C                  (1979), 118-125.
C                (2) BERESFORD N. PARLETT, THE SYMMETRIC EIGENVALUE
C                  PROBLEM, PRENTICE-HALL, ENGLEWOOD CLIFFS, 1980.
C                (3) HEINZ RUTISHAUSER, SIMULTANEOUS ITERATION METHOD FOR
C                  SYMMETRIC MATRICES, NUMER. MATH. 16(1970), 205-223.
C                (4) B.T. SMITH ET AL, MATRIX EIGENSYSTEM ROUTINES -
C                  EISPACK GUIDE, 2-ND ED.,LECTURE NOTES IN COMPUTER
C                  SCIENCE 6, SPRINGER-VERLAG, NEW YORK, 1976.
C***ROUTINES CALLED  IMTQL2,ORTHOG,R1MACH,RANDOM,TRED2,XERRWV
C***END PROLOGUE
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